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(FILE 'HOME' ENTERED AT 14:43:22 ON 22 DEC 2001)

FILE 'CAPLUS' ENTERED AT 14:43:32 ON 22 DEC 2001

E WO 0190106/PN

E WO 200190106/PN

L1 1 S E3

SELECT L1 1 RN

FILE 'REGISTRY' ENTERED AT 14:44:54 ON 22 DEC 2001

31 S E1-31

L3 1 S L2 AND C16H21F2NO2/MF

* *

FILE 'CAOLD' ENTERED AT 14:48:20 ON 22 DEC 2001

L4 0 S L3

FILE 'BEILSTEIN' ENTERED AT 14:48:33 ON 22 DEC 2001

L5 0 S L3

L6 0 S L3 SSS FULL

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L2

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN 8-Azabicyclo[3.2.1]octan-3-one, 8-(phenylmethyl)-, oxime (9CI)

MF C14 H18 N2 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

MF C13 H19 N O2

CI COM

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN Carbamic acid, [(1S)-3-oxo-1-phenylpropyl]-, 1,1-dimethylethyl ester (9CI)

MF C14 H19 N O3

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C27 H39 N5 O

Absolute stereochemistry. Rotation (-).

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C26 H36 F3 N5 O

Absolute stereochemistry. Rotation (-).

$$_{\mathrm{F_{3}C}}$$
 $_{\mathrm{H}}^{\mathrm{Ph}}$ $_{\mathrm{R}}^{\mathrm{N}}$ $_{\mathrm{i-Pr}}^{\mathrm{Me}}$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C29 H40 F3 N5 O

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C22 H30 N2

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C27 H41 N5 O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C27 H40 F N5 O2

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C14 H18 F N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

★ MF C18 H23 F2 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

*

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN Cyclohexanecarboxamide, 4,4-difluoro-N-[(1S)-3-oxo-1-phenylpropyl]- (9CI)

MF C16 H19 F2 N O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C30 H39 N5 O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN Furan, tetrahydro-2,5-dimethoxy- (6CI, 7CI, 8CI, 9CI)

MF C6 H12 O3

CI COM

$$MeO \longrightarrow OMe$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN Benzenemethanamine, hydrochloride (9CI)

MF C7 H9 N . Cl H

CI COM

 H_2N-CH_2-Ph

● HCl

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN Benzenepropanoic acid, .beta.-amino-, methyl ester, (.beta.S)- (9CI)

MF C10 H13 N O2

CI COM

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

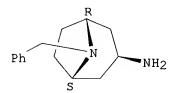
L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN 8-Azabicyclo[3.2.1]octan-3-amine, 8-(phenylmethyl)-, (3-exo)- (9CI)

MF C14 H20 N2

CI COM

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN Cyclohexanecarboxylic acid, 4,4-difluoro- (9CI)

MF C7 H10 F2 O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN Benzenepropanoic acid, .beta.-[[(1,1-dimethylethoxy)carbonyl]amino]-,
methyl ester, (.beta.S)- (9CI)

MF C15 H21 N O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C28 H41 N5 O

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

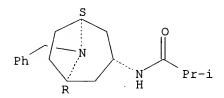
MF C29 H41 F2 N5 O

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C18 H26 N2 O

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

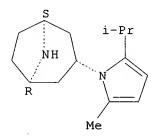
L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C15 H24 N2

CI COM

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C22 H33 N5

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C22 H32 F N5

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN Cyclohexanecarbonyl chloride, 4,4-difluoro- (9CI)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

MF C16 H21 F2 N O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C17 H17 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN INDEX NAME NOT YET ASSIGNED

MF C15 H24 N2 . C7 H8 O3 S

CM 1

Relative stereochemistry.

CM 2

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

IN Benzenepropanoic acid, .beta.-amino-, ethyl ester, (.beta.S)- (9CI)

MF C11 H15 N O2

CI COM

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s 12 and C16H21F2NO2/mf

15 C16H21F2NO2/MF

L3 1 L2 AND C16H21F2NO2/MF

=> d

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS

RN **376348-77-5** REGISTRY

CN Cyclohexanecarboxamide, 4,4-difluoro-N-[(1S)-3-hydroxy-1-phenylpropyl](9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H21 F2 N O2

SR CA

LC STN Files: CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2001 ACS ACCESSION NUMBER: 2001:868452 CAPLUS

TITLE: Preparation of therapeutic tropane derivatives

INVENTOR(S): Perros, Manoussos; Price, David Anthony; Stammen,

Blanda Luzia Christa; Wood, Anthony

PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

INT. PATENT CLASSIF .:

MAIN: C07D451-00

CLASSIFICATION: 31-3 (Alkaloids)

Section cross-reference(s): 1, 63

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND		DATE			APPLICATION NO.				ο.	DATE			
WO	2001090106			A2		20011129			WO 2001-IB806				20010509				
	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	PL,	PT,
		RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,
		UZ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM		
	RW:	GH,	GM,	ΚE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG		
PRIORITY APPLN. INFO.:						GB 2000-14046 A 200005								0526			
						GB 2000-15835 A 2000062							0627				

GRAPHIC IMAGE:

ABSTRACT:

The tropanes I (R1 = C3-6 cycloalkyl optionally substituted by one or more fluorine atoms, C1-6 alkyl optionally substituted by one or more fluorine atoms, C3-6 cycloalkylmethyl optionally ring-substituted by one or more fluorine atoms; R2 = Ph optionally substituted by one or more fluorine atoms) and their pharmaceutically acceptable salts and solvates were prepd. Thus, (1S)-3-[3-(3-isopropyl-5-methyl-4H-1,2,4-triazol-4-yl)-exo-8-azabicyclo[3.2.1]oct-8-yl]-1-phenyl-1-propanamine, prepn. given, was treated with cyclobutanecarboxylic acid in presence of polymer bound N-benzyl-N'-cyclohexylcarbodiimide to give I (R1 = cyclobutyl, R2 = Ph). I had an IC50 value of less than 10nM in the assay for CCR5 binding.

Ι

SUPPL. TERM: tropane deriv prepn CCR5 receptor

INDEX TERM: Respiratory tract (disease; prepn. of tropane derivs. as CCR5 receptor antagonists) INDEX TERM: Intestine, disease (inflammatory; prepn. of tropane derivs. as CCR5 receptor antagonists) INDEX TERM: Anti-AIDS agents Anti-inflammatory agents Crystal structure Molecular structure Respiratory distress syndrome (prepn. of tropane derivs. as CCR5 receptor antagonists) INDEX TERM: Chemokines ROLE: BSU (Biological study, unclassified); BIOL (Biological study) (prepn. of tropane derivs. as CCR5 receptor antagonists) INDEX TERM: Chemokine receptors ROLE: BSU (Biological study, unclassified); BIOL (Biological study) (.beta. chemokine receptor CCR5; prepn. of tropane derivs. as CCR5 receptor antagonists) INDEX TERM: 376348-65-1P ROLE: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of tropane derivs. as CCR5 receptor antagonists) INDEX TERM: 376348-62-8P 376348-63-9P 376348-64-0P 376348-66-2P ROLE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of tropane derivs. as CCR5 receptor antagonists) INDEX TERM: 696-59-3, 2,5-Dimethoxytetrahydrofuran 3082-69-7 3287-99-8, Benzylamine hydrochloride 120686-18-2 122665-97-8 376348-71-9 376348-74-2 ROLE: RCT (Reactant); RACT (Reactant or reagent) (prepn. of tropane derivs. as CCR5 receptor antagonists) INDEX TERM: 28957-72-4P 37088-66-7P 76272-34-9P 76272-36-1P 135865-78-0P 190189-97-0P 376348-67-3P 376348-68-4P 376348-69-5P 376348-70-8P 376348-72-0P 376348-73-1P 376348-75-3P 376348-76-4P **376348-77-5P** 376348-78-6P 376348-79**-**7P 376348-80-0P 376348-81-1P ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of tropane derivs. as CCR5 receptor antagonists)

